

Effects of nonintegrability on stabilization of Feshbach molecules in atom waveguides

V. A. Yurovsky

School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel

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Deactivation of broad quasi-one-dimensional dibosonic molecules is analyzed. Within integrable Lieb-Liniger-McGuire (LLMG) model an exact expression does not demonstrate suppression of the deactivation at low collision energies. Solution of Faddeev equations demonstrates that when a Feshbach resonance lifts the symmetry of the LLMG model the deactivation becomes suppressed. This effect shows a way for formation of a stable gas of dibosonic Feshbach molecules.

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Ultracold molecules have recently been formed by Feshbach resonance association (see reviews [1] and original works [2, 3]). These Feshbach molecules are very broad since they are superpositions of the closed and open channels. However, inelastic collisions of atoms and molecules lead to strong losses of molecules composed from Bose atoms in experiments [2]. In the fermionic case [3] inelastic collisions are strongly suppressed due to Pauli blocking and weak coupling of the atoms [4]. This effect allows investigation of BEC-BCS crossover and other phenomena of fundamental physical importance.

Tight confinement of atomic motion in two directions by atom waveguides strongly modifies atomic collisions in quasi-one-dimensional (1D) regime, when the transverse excitation energy ω_{\perp} (in units where $\hbar = 1$) substantially exceeds the collision energies [5]. This regime has been realized in 2D optical lattices [6, 7], elongated atomic traps [8], and atomic integrated optics devices [9]. Broad quasi-1D molecules, predicted in [10] and observed in [7], have binding energies less than ω_{\perp} . Such diatoms can be described by two-channel 1D model [11, 12], where the closed channel incorporates both 3D closed channel and excited transverse waveguide modes.

Rates of deactivation into tightly bound (non-Feshbach) states are approximately proportional to the probability to find three atoms (two of which belong to the molecule) in the same place, e. g. to three-body (3B) correlations [4]. 3B correlations were analyzed in [13] within exactly-soluble Lieb-Liniger model [14]. In this model 1D bosons interact by zero-range potentials $U_a \delta(z_j - z_l)$, where z_j are atomic coordinates and the interaction strength U_a is energy-independent. In the case of repulsive interactions ($U_a > 0$), which does not bound the atoms, the correlations are suppressed at low collision energies and strong interactions [13]. Bound states can be formed in the case of attractive interactions ($U_a < 0$) described by the McGuire solution [15]. The tree-atom correlations for atom and diatom with relative momentum p_0 can be represented, using 3B wavefunction $\varphi_0(z_1, z_2, z_3)$ [15], as

$$|\varphi_0(0, 0, 0)|^2 = \frac{m|U_a|}{24\pi^2} \frac{9p_0^2 + m^2 U_a^2}{p_0^2 + m^2 U_a^2}, \quad (1)$$

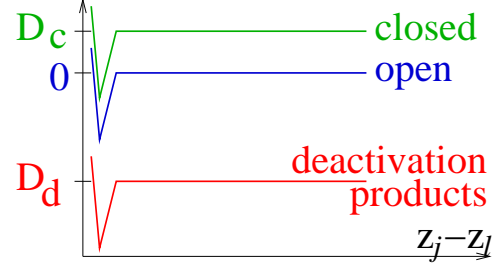


FIG. 1: Schematic description of 2B channel potentials.

where m is the atomic mass. This expression has a non-zero limit at low collision energies ($p_0 \rightarrow \infty$) or strong interactions ($|U_a| \rightarrow \infty$). This behavior differs from the free-atom case [13], since bound atoms keep non-vanishing imaginary momenta $\pm \frac{i}{2} m U_a$ even when $p_0 \rightarrow 0$. Thus, inelastic collisions of 1D broad molecules are cardinally different from collisions of two structureless particles, which are suppressed both within the Lieb-Liniger-McGuire (LLMG) model [13] and beyond it [16]. This difference reflects the fact that broad Feshbach molecules can not be considered as zero-range objects and their deactivation is not a 2B process.

The present Letter demonstrates that deactivation of broad 1D molecules becomes suppressed when integrability of LLMG model is lifted by a Feshbach resonance. Similar effects can be expected for other mechanisms of integrability lifting, e. g. due to virtual transverse mode excitation [18, 19]. In contrast with these effects, other processes, such as reflection and dissociation in atom-diatom collisions and three-atom association [17], become allowed when the nonintegrability is lifted.

Except of demonstration of a new observable effect of non-integrability, which is interesting for atomic, molecular, and statistical physics, as well as for quantum field theory, present results show a way for formation of a stable gas of dibosonic Feshbach molecules.

Consider multichannel collisions of 1D Bose atoms described by the annihilation operators $\hat{\Psi}_a(z)$. The model includes several 2B channels (see Fig. 1). The Feshbach closed-channel state, described by the molecular annihilation operator $\hat{\Psi}_c(z)$, lies at the energy D_c close to the

open channel threshold, which serves as the energy origin. A set of deactivation product channels $\{d\}$, described by the molecular annihilation operators $\hat{\Psi}_d(z)$, lie at the energies D_d far below the open channel threshold. The system can be described by the Hamiltonian

$$\begin{aligned} \hat{H} = & \int dz \left\{ \hat{\Psi}_a^\dagger(z) \left[-\frac{1}{2m} \frac{\partial^2}{\partial z^2} + \frac{U_a}{2} \hat{\Psi}_a^\dagger(z) \hat{\Psi}_a(z) \right] \hat{\Psi}_a(z) \right. \\ & + \sum_{j=c,\{d\}} \hat{\Psi}_j^\dagger(z) \left(-\frac{1}{4m} \frac{\partial^2}{\partial z^2} + D_j \right) \hat{\Psi}_j(z) + \hat{V}_{\text{Fesh}}(z) \\ & \left. + \hat{V}_{\text{Fesh}}^\dagger(z) + \sum_{\{d\}} \left[\hat{V}_{ad}(z) + \hat{V}_{ad}^\dagger(z) + \hat{V}_{cd}(z) + \hat{V}_{cd}^\dagger(z) \right] \right\}. \quad (2) \end{aligned}$$

Here the interaction $\hat{V}_{\text{Fesh}}(z) = g \hat{\Psi}_c^\dagger(z) \hat{\Psi}_a(z) \hat{\Psi}_a(z)$ describes the Feshbach coupling, and

$$\hat{V}_{ad}(z) = d_{ad} \hat{\Psi}_a^\dagger(z) \hat{\Psi}_a^\dagger(z) \hat{\Psi}_d(z), \quad \hat{V}_{cd}(z) = d_{cd} \hat{\Psi}_c^\dagger(z) \hat{\Psi}_d(z) \quad (3)$$

are couplings of the open and closed channels, respectively, to the product channels. The non-resonant interaction strength U_a , resonance detuning D_c , and the Feshbach coupling strength g can be related to parameters of atomic collisions and the waveguide [11, 12] [see Eq. (15) below].

Like in the two-channel case [17], 2B problem can be described by the 1D T matrix

$$T_{1D}(k) = \left[U_{\text{eff}}^{-1}(k^2/m) + \frac{i}{2} m k^{-1} \right]^{-1}, \quad (4)$$

which depends on the relative momentum k of two colliding atoms, where the energy-dependent interaction strength $U_{\text{eff}}(E_c)$ incorporates effects of all channels. The poles of $T_{1D}(k)$ on the positive imaginary axis, $k = i\kappa_n$, correspond to 2B bound states (diatoms) with energies $-\kappa_n^2/m$. They are superpositions of the open, closed, and deactivation product channels. The diatoms have finite size ($\sim \kappa_n^{-1}$), although this model approximates the closed-channel and the deactivation-product molecules to be infinitesimal in size.

Substitution of the state vector for the three-atom system

$$\begin{aligned} |\Psi_3\rangle = & \left\{ \frac{1}{\sqrt{6}} \int d^3z \varphi_0(z_1, z_2, z_3) \hat{\Psi}_a^\dagger(z_1) \hat{\Psi}_a^\dagger(z_2) \hat{\Psi}_a^\dagger(z_3) \right. \\ & \left. + \sum_{j=c,\{d\}} \int dz dz_m \varphi_d(z, z_m) \hat{\Psi}_a^\dagger(z) \hat{\Psi}_d^\dagger(z_m) \right\} |\text{vac}\rangle, \quad (5) \end{aligned}$$

where $|\text{vac}\rangle$ is the vacuum state, into stationary Schrödinger equation with the Hamiltonian (2) leads to coupled equations for the wavefunctions of the open (three-atom) channel $\varphi_0(z_1, z_2, z_3)$, the closed (atom-molecule) $\varphi_c(z, z_m)$, and the product channels $\varphi_d(z, z_m)$. Elimination of the closed and product channels (like in [12, 17]) results in a single equation for

$\varphi_0(z_1, z_2, z_3)$, which can be reduced to the Faddeev-Lovelace equation for the symmetric transition amplitude $X(p, p_0)$,

$$\begin{aligned} X(p, p_0) = & 2Z(p, p_0) + \frac{m^2}{2\kappa_0^3} \int dq Z(p, q) T_{1D}(k(q)) X(q, p_0) \\ Z(p, q) = & \frac{2\kappa_0^3}{\pi m} \frac{1}{mE + i0 - p^2 - pq - q^2}. \quad (6) \end{aligned}$$

Here $k(q) = \sqrt{mE + i0 - 3q^2/4}$, E is the total energy in the center-of-mass system, $p_n = 2\sqrt{(mE + \kappa_n^2)/3}$ is the relative momentum of the atom and diatom in the state n , and $n = 0$ corresponds to the initial diatom state. The probabilities of inelastic reflection and transmission with the diatom transition to the state $n \neq 0$ can be expressed as

$$P_{\text{ref, tr}}(0 \rightarrow n) = \frac{16\pi^2}{9} \frac{m^2 W_0 W_n}{p_0 p_n} \left(\frac{\kappa_n}{\kappa_0} \right)^3 |X(\mp p_n, p_0)|^2, \quad (7)$$

where $\kappa_0 < \kappa_n$ and W_n is the contribution of the open channel into the diatom state n (see [12, 17]). The deactivation rate coefficient is

$$K_{1D} = \frac{3p_0}{2m} \sum_{n \neq 0} [P_{\text{ref}}(0 \rightarrow n) + P_{\text{tr}}(0 \rightarrow n)]. \quad (8)$$

In the case of high deactivation energies,

$$|D_d| \gg \max(|d_{cd}^2/D_c|, |d_{ad}d_{cd}/g|, |d_{ad}^2/U_a|, |E|, |D_c|, mU_a^2), \quad (9)$$

$T_{1D}(k)$ has poles at $k = i\kappa_d \approx i\sqrt{m|D_d|}$, corresponding to the deactivation products. Other poles are approximately determined by the same cubic equation as in the two-channel model [17, 20],

$$\kappa^3 + \frac{m}{2} U_a \kappa^2 + m D_c \kappa + \frac{1}{2} m^2 D_c U_a - m^2 |g|^2 = 0. \quad (10)$$

Contributions of the product channels into the corresponding weaker-bound diatoms ($\kappa_n \ll \kappa_d$, $n \neq d$) can be neglected. Whenever $U_a > 0$ or $D_c > 2|g|^2/U_a$, when Eq. (10) has a single real positive root, the deactivation rate coefficient can be approximately expressed as

$$K_{1D} = \sum_{\{d\}} |\gamma_{ad} \varphi_0(0, 0, 0) + \gamma_{cd} \varphi_c(0, 0)|^2 \quad (11)$$

in terms of the wavefunctions of the open and closed channels in the origin

$$\begin{aligned} \varphi_0(0, 0, 0) = & \frac{\sqrt{3W_0\kappa_0}}{2\pi} \left[1 + \frac{im^2}{4\kappa_0^2} \int dq \frac{T_{1D}(k(q)) X(q, p_0)}{k(q)} \right] \\ \varphi_c(0, 0) = & -\frac{mg}{\pi} \sqrt{\frac{W_0\kappa_0}{2}} \left[\frac{1}{\kappa_0^2 + mD_c} \right. \\ & \left. + \frac{m}{2\kappa_0^2} \int dq \frac{T_{1D}(k(q)) X(q, p_0)}{U_a(k^2(q) - mD_c) + 2m|g|^2} \right]. \end{aligned}$$

Here the transition amplitude $X(q, p_0)$ is a solution of Eqs. (6) with $T_{1D}(k)$ (4), where the energy-dependent interaction strength is approximated by

$$U_{\text{eff}}(E_c) = U_a + \frac{2|g|^2}{E_c + i0 - D_c}, \quad (12)$$

of the two-channel model [17].

The coefficients in Eq. (11) are expressed as

$$\gamma_{ad} = \left(\frac{3^5 4m}{|D_d|^5} \right)^{1/4} |d_{da}| U_a, \quad \gamma_{cd} = 2 \left(\frac{3^3 m}{|D_d|^5} \right)^{1/4} |d_{da}| g^*. \quad (13)$$

The same deactivation rate can be obtained within another model, assuming deactivation due to three-atom interactions,

$$\hat{V}_{ad}(z) = \frac{1}{4\pi} \left(\frac{|D_d|}{3m} \right)^{1/4} \gamma_{ad} \hat{\Psi}_a^\dagger(z) \hat{\Psi}_a^\dagger(z) \hat{\Psi}_a^\dagger(z) \hat{\Psi}_a(z) \hat{\Psi}_d(z) |\varphi_0(0,0,0)|^2$$

$$\hat{V}_{cd}(z) = \frac{1}{4\pi} \left(\frac{3|D_d|}{4m} \right)^{1/4} \gamma_{cd} \hat{\Psi}_c^\dagger(z) \hat{\Psi}_a^\dagger(z) \hat{\Psi}_a(z) \hat{\Psi}_d(z) |\varphi_c(0,0)|^2 \quad (14)$$

in place of two-atom ones (3).

If the non-resonant case ($g = 0$, $\varphi_c = 0$) the problem is reduced to the LLMG model [14, 15], which has an exact Bethe-ansatz solution. In agreement with [4], K_{1D} of Eq. (11) is proportional to the three-atom correlations (1), which does not describe suppression of deactivation.

A physical sense of this effect can be explained by a simple 2B analogy. Consider a collision of 1D atom and molecule with coordinates y and x , respectively. The wavefunction of this system has the form of $\varphi(y, x) = \exp(ip_0(y - x)) + R \exp(ip_0|y - x|)$, where R is the reflection amplitude. In the LLMG model atom-diatom reflection is forbidden, $R = 0$, and the 2B analogy leads to $\varphi(0,0) = 1 + R = 1$. The 3B model results in Eq. (1), which has a non-zero value too since the three atoms can approach each other.

However, reflection becomes allowed when integrability of the LLMG model is lifted e.g. by a Feshbach resonance [17]. Moreover, reflection becomes the dominant channel at low collision energy, preventing approaching of the atoms and leading to suppression of deactivation.

This hypothesis is confirmed by numerical calculations. As the coefficients γ are independent of the collision energy and resonance detuning in both models, (3) and (14), the behavior of the deactivation rate (11) is determined by the three-atom correlations for the open $|\varphi_0(0,0,0)|^2$ and closed $|\varphi_c(0,0)|^2$ channels, see Fig. 2. The results are expressed in terms of dimensionless parameters: the non-resonant interaction strength u , the collision energy $\epsilon_2 = 3p_0^2/(4mD_0)$, and the detuning b , where D_0 is the energy scale. In the quasi-1D regime, when $p_0^2/m \ll \omega_\perp$ and the 3D elastic scattering length a_{3D} does not exceed the transverse waveguide

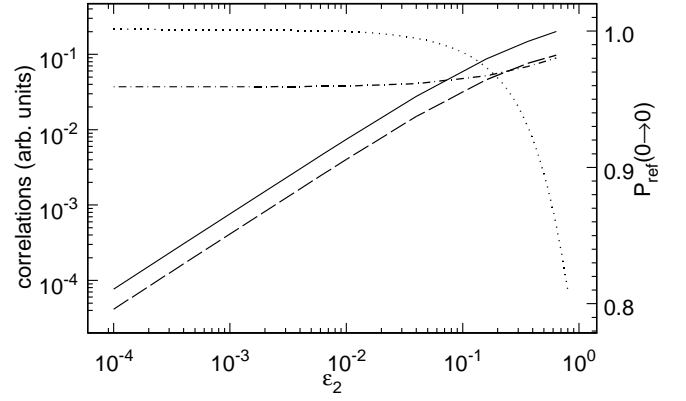


FIG. 2: Three-atom correlations for the open $|\varphi_0(0,0,0)|^2$ (dashed line) and closed $|\varphi_c(0,0)|^2$ (solid line) channels, as well as the elastic reflection probability $P_{\text{ref}}(0 \rightarrow 0)$ (dotted line), calculated as functions of the scaled collision energy ϵ_2 for $U_a = 0$ and $D_c = 0$. The dot-dashed line displays correlations $|\varphi_0(0,0,0)|^2$ within the LLMG model.

length $a_\perp = [2/(m\omega_\perp)]^{1/2}$, the parameters can be expressed as [12]

$$D_0 = m^{1/3}|g|^{4/3} = m^{1/3}(\omega_\perp a_{3D}\mu\Delta)^{2/3} \beta_1^{-4/3} \beta_2^{2/3}$$

$$u = m^{1/3}|g|^{-2/3}U_a = 2(m\omega_\perp^2 a_{3D}^2)^{1/3} (\beta_1\beta_2\mu\Delta)^{-1/3} \quad (15)$$

$$b = D_c/D_0 = [\mu(B - B_0) - \omega_\perp + Ca_{3D}\mu\Delta/(\beta_1 a_\perp)]/D_0,$$

with $\beta_1 = 1 - Ca_{3D}/a_\perp$ and $\beta_2 = 1 + C'a_{3D}\mu(B - B_0 - \Delta - \omega_\perp/\mu)^2/(2a_\perp\omega_\perp\Delta)$. Here Δ is the phenomenological resonance strength, μ is the difference between the magnetic momenta of an atomic pair in the open and closed channels, $B - B_0$ is the detuning of the external magnetic field B from its resonant value B_0 , $C \approx 1.4603$ [5], and $C' \approx 1.3062$ [12]. For example, in a waveguide with the transverse frequency $\omega_\perp = 50 \times 2\pi$ KHz, collisions remain quasi-1D for the collision energy less than $2.4\mu\text{K}$. In vicinity of $b = 0$, Eq. (15) gives $D_0 = 3\mu\text{K}$, $u = 0.024$, and $dB/db = 34$ mG for the Na resonance at 907 G and $D_0 = 2.5\mu\text{K}$, $u = 0.12$, and $dB/db = 27$ mG for the ^{87}Rb resonance at 1007 G. Figure 2 demonstrates that the correlations and, therefore, the deactivation rate K_{1D} decrease proportionally to the collision energy for slow collisions, when the total elastic reflection is approached. It is surprising that non-integrability leads to the same low-energy behavior of deactivation rate of broad molecules as in collisions of structureless particles [13, 16]. At rather high collision energy, when the elastic reflection probability decreases, correlations in the open channel follow to the LLMG model. Deactivation suppression persists in a wide range of the resonance detunings and the non-resonant interaction strengths (see Fig. 3).

The foregoing results are related to high deactivation energies $|D_d|$. The case of low deactivation energies can be considered within the two-channel model [17]. A Fes-

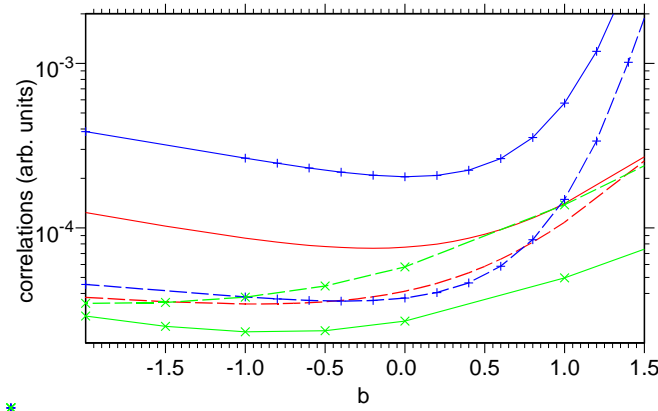


FIG. 3: Three-atom correlations for the open $|\varphi_0(0,0,0)|^2$ (dashed lines) and closed $|\varphi_c(0,0)|^2$ (solid lines) channels, calculated as functions of the scaled detuning for $\epsilon_2 = 1 \times 10^{-4}$ and $u = 1$ (pluses), $u = -1$ (crosses), and $u = 0$ (no symbols).

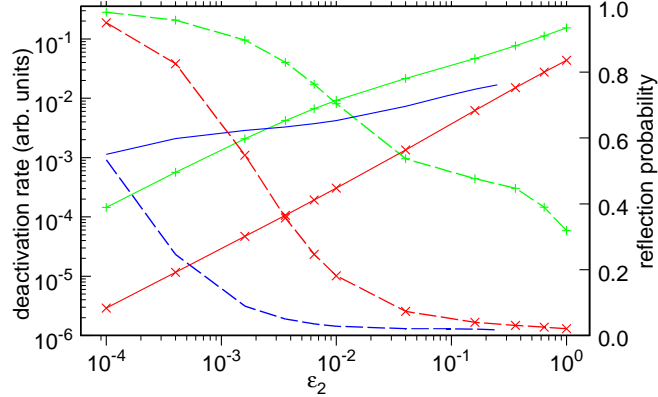


FIG. 4: Deactivation rate coefficient K_{1D} (solid lines) and elastic reflection probability $P_{\text{ref}}(0 \rightarrow 0)$ (dashed lines), calculated as functions of the scaled collision energy ϵ_2 for $b = 0.4$, $u = 10$ (crosses), $b = -2$, $u = -2$ (pluses), and $b = -4$, $u = -1$ (no symbols), within the two-channel model.

hbach molecule can have two bound states at $U_a < 0$ and $D_c < 2|g|^2/U_a$, when Eq. (10) has two real positive solutions, $\kappa_1 > \kappa_0$. Collision with third atom can lead to transitions between the corresponding states, and foreign deactivation product states are not more necessary. This case is exactly described by Eqs. (4), (6), (7) and (12). The deactivation rate is given by Eq. (8), which includes now a single term ($n = 1$) only. It is again proportional to the collision energy for slow collisions (see Fig. 4). Deactivation suppression correlates with the increase in the elastic reflection probability in this model too.

In summary, the integrable LLMG model does not predict suppression of deactivation of broad 1D molecules, demonstrating their difference from compact molecules. The deactivation becomes suppressed when the symmetry of LLMG model is lifted by Feshbach resonance. This effect is predicted by the two-channel model, as well as by two multichannel models with different interactions, (3)

and (14). Dibosonic Feshbach molecules in atom waveguides become thus relatively stable, like difermionic ones in free space. Thus, both the presence [17] and suppression of certain processes are among the observable effect of non-integrability.

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